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Long-time energy conservation of numerical integrators

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This article discusses the energy conservation of a wide class of numerical integrators applied to Hamiltonian systems. It surveys known material by various illustrations, and it also contains more recent and new results.

1.1 Introduction

In this introductory section we present the class of differential equations considered (Hamiltonian systems) together with properties of their flow, and we introduce numerical integration methods that can be expressed as B-series. We further discuss difficulties that can arise when one tries to conserve exactly the Hamiltonian.

1.1.1 Properties of Hamiltonian systems

We consider Hamiltonian systems

$$\begin{aligned} \dot{p} &= -\nabla_q H(p,q) \\ \dot{q} &= \nabla_p H(p,q) \end{aligned} \quad \text{or} \quad \dot{y} = J^{-1}\nabla H(y), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \quad (1.1)$$

where $y = (p,q)^T$ and $H(y) = H(p,q)$ is a real-valued smooth function, and we emphasise the following two properties of such systems:

(P1)   energy conservation, and
(P2)   symplecticity.

Property (P1) just means that $H(y) = H(p,q)$ is constant along solutions of the differential equation. For classical mechanical systems, where $H(p,q) = \frac{1}{2}p^T M(q)^{-1} p + U(q)$ is the sum of kinetic and potential energy, this is equivalent to the conservation of the total energy.

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Property (P2) – symplecticity – can be conveniently expressed in terms of the flow $\varphi_t(y_0)$ of the differential equation, which is the solution at time t for the initial value $y(0) = y_0$. Symplecticity then means that

$$\varphi'_t(y)^T J \varphi'_t(y) = J, \tag{1.2}$$

where prime indicates the derivative with respect to y. It is interesting to mention that this property is characteristic for Hamiltonian systems.

1.1.2 B-series integrators

For a general differential equation $\dot{y} = f(y)$, the Taylor series of the exact solution with initial value $y(0) = y$ can be written as

$$
\begin{aligned}
y(h) \;=\; & y + hf(y) + \frac{h^2}{2!}f'(y)f(y) \\
& + \frac{h^3}{3!}\Big(f''(y)\big(f(y), f(y)\big) + f'(y)f'(y)f(y)\Big) + \ldots
\end{aligned}
\tag{1.3}
$$

We consider numerical integrators $y_{n+1} = \Phi_h(y_n)$, whose Taylor series have the same structure as (1.3) with additional real coefficients:

$$
\begin{aligned}
\Phi_h(y) \;=\; & y + ha(\,\bullet\,)f(y) + h^2 a(\,{\textstyle\uparrow}\,)f'(y)f(y) \\
& + h^3 \Big(\tfrac{a(\vee)}{2}f''(y)\big(f(y), f(y)\big) + a(\,{\textstyle\uparrow}\,)f'(y)f'(y)f(y)\Big) + \ldots
\end{aligned}
\tag{1.4}
$$

The coefficients $a(\tau)$, which are in a one-to-one correspondence with rooted trees, characterise the integrator. Properties like energy conservation and symplecticity can be expressed in terms of these coefficients. Series expansions of the form (1.4), called B-series, have their origin in the paper of Butcher (1972) and were introduced by Hairer & Wanner (1974).

Such B-series integrators are comprised of Runge–Kutta methods (RK), Taylor series methods, the underlying one-step method (in the sense of Kirchgraber (1986), see also chapter XIV of HLW02†) of linear multistep methods (lmm), and all their extensions such as general linear methods (glm) and multistep-multistage-multiderivative methods (mmm); see the left cube of Figure 1.1.

For the numerical treatment of Hamiltonian systems, partitioned methods that allow one to treat the p and q components in a different manner are even more important. The basic method is the symplectic Euler discretisation, which combines the explicit and implicit Euler methods.

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† The monograph "Geometric Numerical Integration" of Hairer, Lubich & Wanner (2002) will be cited frequently. Reference to it will be abbreviated by HLW02.
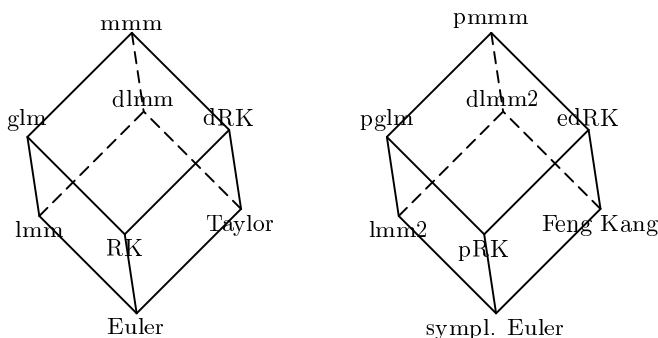
Fig. 1.1. The cube of B-series methods (left) and its extension to partitioned methods (right).

Taylor series methods are replaced by the generating function methods of Feng Kang, multistep methods by their variants for second-order differential equations (lmm2), etc.; see the right cube of Figure 1.1.

1.1.3 Exact energy conservation

For a numerical solution obtained by $y_{n+1} = \Phi_h(y_n)$ we would like to have energy conservation (i.e., $H(y_n) = const$ for all n) and symplecticity (i.e., $\Phi_h'(y)^T J \Phi_h'(y) = J$) at the same time. Unfortunately, this is not possible. Ge & Marsden (1988) proved that for Hamiltonian systems without further conserved quantities such a method has to be a re-parametrisation of the exact flow. An algebraic proof for the impossibility of having an energy conserving symplectic B-series integrator (which is different from the exact flow) is given by Chartier, Faou & Murua (2005).

Let us study what happens when we force energy conservation and thus give up symplecticity. We consider the three-body problem (Sun–Jupiter–Saturn) which is a Hamiltonian system with

$$H(p, q) = \frac{1}{2} \sum_{i=0}^{2} \frac{1}{m_i} p_i^T p_i - G \sum_{i=1}^{2} \sum_{j=0}^{i-1} \frac{m_i m_j}{\|q_i - q_j\|}.$$

The initial values $q_i(0), p_i(0) \in \mathbf{R}^3$ and the parameters G and m_i are taken from HLW02, page 11. To this problem we apply two kinds of integrators that exactly conserve the Hamiltonian along the numerical solution. Notice, however, that neither of these methods is symmetric so that the considerations of Section 1.4 do not apply.
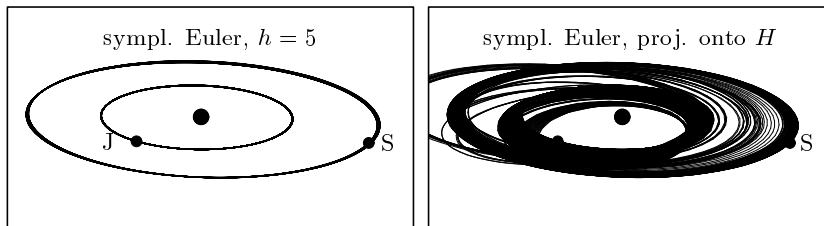
Fig. 1.2. Numerical solution of the Sun–Jupiter–Saturn system.

Projection method. The most obvious approach for achieving exact energy conservation is by projection. Assume that y_n is an approximation to $y(t_n)$ satisfying $H(y_n) = H(y_0)$. We compute $\widehat{y}_{n+1} = \Phi_h(y_n)$ with some basic method, and then project $\widehat{y}_{n+1}$ orthogonally onto the energy surface $\{y \,|\, H(y) = H(y_0)\}$ yielding y_{n+1}. If we take as basic method the symplectic Euler method (see method (1.8) below), an integration with step size $h = 5$ over an interval of $1.3 \cdot 10^6$ Earth days gives the result of Figure 1.2. The left picture shows the numerical solution obtained without any projection. Although the energy is not exactly conserved, we observe a qualitatively correct behaviour (for an explanation see Section 1.2). The picture on the right in Figure 1.2 shows the result obtained by the same method, but with an additional projection onto the energy surface after every step. Clearly, this does not improve the result; in fact, it even destroys the good long-time behaviour.

Energy conserving B-series method. In the previous experiment one can criticise the fact that the projection step throws out the method from the class of B-series integrators. This is correct. Motivated by the results of Faou, Hairer & Pham (2005) we therefore consider the method $y_{n+1} = \Phi_h(y_n)$, where $\Phi_h(y)$ is the exact flow at time $t = h$ of

$$\dot{y} = f(y) + h^3 \big(f' f''(f, f) + f''(f, f' f) \big)(y). \qquad (1.5)$$

It is not difficult to check that this is a B-series method, and that for $f(y) = J^{-1} \nabla H(y)$ the energy $H(y)$ is a first integral of (1.5), so that $H(y_n) = const$. Since the perturbation in (1.5) is not Hamiltonian, the method is not symplectic. We do not claim that this method can be realised by a Runge–Kutta or multistep method. Application to the Sun–Jupiter–Saturn system gives a result that is very similar to that of the projection method (right picture of Figure 1.2).

From these experiments we conclude that exact energy conservation

alone is certainly not sufficient for a qualitatively correct long-time integration of Hamiltonian systems.

1.2 Methods that exactly conserve quadratic first integrals

We now turn our attention to property (P2) – symplecticity – of Hamiltonian systems. This turns out to be closely related to the exact conservation of quadratic first integrals.

1.2.1 Equivalence with symplecticity

Consider the Hamiltonian system together with its variational equation,

$$\dot{y} = J^{-1}\nabla H(y), \qquad \dot{\Psi} = J^{-1}\nabla^2 H(y)\Psi, \tag{1.6}$$

where $\Psi(t)$ is the derivative of $y(t)$ with respect to its initial value. The symplecticity condition (1.2) just expresses the fact that $\Psi^T J \Psi$ is a first integral of the system (1.6); i.e., it is constant along solutions of (1.6).

Theorem 1.2.1 (criterion for symplecticity) *A B-series integrator is symplectic (i.e., it satisfies $\Phi'_h(y)^T J \Phi'_h(y) = J$) if and only if it exactly conserves all quadratic first integrals of a system $\dot{y} = f(y)$.*

Conservation of quadratic first integrals implies symplecticity. Bochev & Scovel (1994) have shown for Runge–Kutta and general linear methods that the derivative of the numerical solution with respect to the initial value, $\Psi_n := \partial y_n/\partial y_0$, is the result of the same numerical method applied to the augmented system (1.6). This implies the statement, because $\Psi^T J \Psi$ is a quadratic first integral of the system. The extension to B-series methods is straight-forward.

Symplecticity implies conservation of quadratic first integrals. Calvo & Sanz-Serna (1994) have given a characterisation of the symplecticity of B-series methods in terms of the coefficients $a(\tau)$ of (1.4); see also HLW02, page 201. Chartier, Faou & Murua (2005) show that exactly the same conditions on the coefficients imply that the method conserves exactly all quadratic first integrals of the differential equation.

Implicit midpoint rule. Let us illustrate the above characterisation of symplectic B-series methods for the implicit midpoint rule

$$y_{n+1} - y_n = hf\big((y_{n+1} + y_n)/2\big). \tag{1.7}$$

For this we assume that $Q(y) = y^T C y$ (with a symmetric matrix C) is a first integral of $\dot{y} = f(y)$, i.e., $y^T C f(y) = 0$ for all y. Left-multiplication of (1.7) with $(y_{n+1} + y_n)^T C$ yields a vanishing right-hand side and

$$0 = (y_{n+1} + y_n)^T C(y_{n+1} - y_n) = y_{n+1}^T C y_{n+1} - y_n^T C y_n.$$

This proves that $Q(y_n)$ is exactly conserved, implying that the implicit midpoint rule is a symplectic integrator.

1.2.2 Partitioned methods

As mentioned in the introduction, partitioned methods play an important role for solving Hamiltonian systems. They allow one to treat the variables p and q in the Hamiltonian system (1.1) in a different way. For partitioned methods the above characterisation remains valid only if one restricts the statements to quadratic first integrals of the special form $Q(p, q) = p^T E q$ with an arbitrary matrix E.

Symplectic Euler method. Consider the combination of the implicit and explicit Euler methods. This yields the discretisation

$$
\begin{aligned}
p_{n+1} &= p_n - h \nabla_q H(p_{n+1}, q_n) \\
q_{n+1} &= q_n + h \nabla_p H(p_{n+1}, q_n).
\end{aligned}
\tag{1.8}
$$

If $p^T E q$ is a first integral of (1.1), a multiplication of the first relation of (1.8) by $(E q_n)^T$, of the second relation by $p_{n+1}^T E$, and addition of the two proves the exact conservation of this first integral. Consequently, the method is symplectic.

Störmer–Verlet scheme. Composing a half-step of method (1.8) with its adjoint (explicit in p and implicit in q) gives

$$
\begin{aligned}
p_{n+1/2} &= p_n - \frac{h}{2} \nabla_q H(p_{n+1/2}, q_n) \\
q_{n+1} &= q_n + \frac{h}{2} \Big(\nabla_p H(p_{n+1/2}, q_n) + \nabla_p H(p_{n+1/2}, q_{n+1}) \Big) \\
p_{n+1} &= p_{n+1/2} - \frac{h}{2} \nabla_q H(p_{n+1/2}, q_{n+1}).
\end{aligned}
\tag{1.9}
$$

As the composition of symplectic mappings it is a symplectic integrator.

For a separable Hamiltonian $H(p, q) = p^T p / 2 + U(q)$, this scheme implies

$$q_{n+1} - 2q_n + q_{n-1} = -h^2 \, \nabla_q U(q_n), \tag{1.10}$$

which is a natural discretisation of $\ddot{q} = -\nabla_q U(q)$ that can already be found in the Principia of Newton; c.f., Hairer, Lubich & Wanner (2003).

1.2.3 Near energy conservation

The aim of this article is to study energy conservation of numerical integrators. In general, symplectic B-series methods cannot conserve the Hamiltonian exactly (see Section 1.1.3). However, we have the following central result, which was intuitively clear since the use of symplectic methods and was rigorously proved by Benettin & Giorgilli (1994); see also Section IX.8 of HLW02.

Theorem 1.2.2 *Consider*

- *a Hamiltonian system with analytic $H : U \to \mathbf{R}$, and*
- *a symplectic B-series method $\Phi_h(y)$ of order r.*

As long as $\{y_n\}$ stays in a compact set, we have for $t_n = nh$ and $h \to 0$,

$$H(y_n) = H(y_0) + \mathcal{O}(h^r) + \mathcal{O}(t_n e^{-\gamma/\omega h}), \qquad (1.11)$$

where $\gamma > 0$ only depends on the method, and ω is related to the Lipschitz-constant (or highest frequency) of the differential equation.

If h is small enough, the second error term in (1.11) is exponentially small on exponentially long time intervals. Thus we have error conservation up to a bounded $\mathcal{O}(h^r)$ term on such long intervals.

Let us illustrate this behaviour with the symplectic Euler method (1.8) applied to the Sun–Jupiter–Saturn system. Figure 1.3 shows the relative error in the Hamiltonian on an interval of 500 000 Earth days. The energy oscillates around the correct constant value and does not show any drift. The non-symplectic explicit Euler method, however, has a linear drift in the energy that makes the method useless even when applied with a much smaller step size.
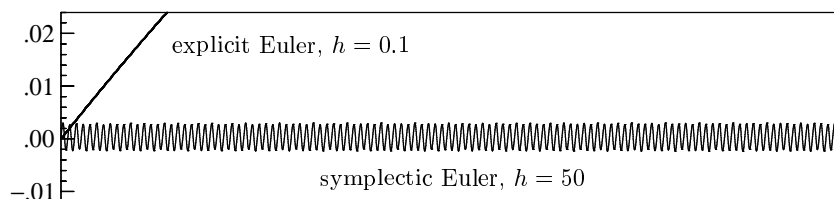

Fig. 1.3. Energy conservation of numerical methods.

Idea of the proof (backward error analysis). Let us indicate the proof of the previous theorem. This is a welcome opportunity for mentioning backward error analysis which is one of the most important tools in the analysis of geometric integrators.

Formal analysis.   The numerical solution of a B-series method can be interpreted as the exact solution of a modified differential equation which, very similar to (1.4), is of the form

$$
\begin{aligned}
\dot{y} &= f(y) + h b(\,\centerdot\!\!\centerdot\,) f'(y) f(y) \\
&+ h^2 \Big(\tfrac{b(\!\vee\!)}{2} f''(y)\big(f(y), f(y)\big) + b(\,\centerdot\!\!\centerdot\!\!\centerdot\,) f'(y) f'(y) f(y) \Big) + \dots
\end{aligned}
\tag{1.12}
$$

The coefficients $b(\tau)$ of this modified equation are obtained recursively by comparing the series (1.4) with the Taylor series expansion of the solution of (1.12) at $t = h$. Consequently, we have $y_n = \widetilde{\varphi}_{nh}(y_0)$, where $\widetilde{\varphi}_t(y)$ is the exact flow of (1.12).

It turns out that for symplectic B-series integrators (1.4) and for $f(y) = J^{-1} \nabla H(y)$, (1.12) is Hamiltonian with modified Hamiltonian

$$
\widetilde{H}(y) = H(y) + h^r H_{r+1}(y) + h^{r+1} H_{r+2}(y) + \dots
\tag{1.13}
$$

Since the exact flow $\widetilde{\varphi}_t(y)$ conserves the Hamiltonian $\widetilde{H}(y)$, it follows that $\widetilde{H}(y_n) = const$, and thus $H(y_n) = H(y_0) + \mathcal{O}(h^r)$. Unfortunately, the above series are asymptotic series and usually diverge. This is why we call this part of the proof a *formal analysis*.

Rigorous analysis.   Whereas the formal analysis is relatively simple and gives already much insight into long-time integration, the rigorous analysis is rather technical. One has to truncate the series so that the resulting error in $y_n - \widetilde{\varphi}_{nh}(y_0)$ is as small as possible. This induces the linearly increasing exponentially small error term in the statement of Theorem 1.2.2.

Illustration with the Lennard–Jones potential. To illustrate the result of the previous theorem, consider the Hamiltonian

$$
H(p, q) = \frac{1}{2} p^2 + q^{-12} - q^{-6},
$$

which models the motion of a particle against a strongly repelling wall. The variable q represents the distance to the wall, and p the velocity of the particle. With initial values $q_0 = 10$ and $p_0 < 0$ such that $H(p_0, q_0) = 1$, the particle moves against the wall until $t \approx 6.5$, and then it bounces off.
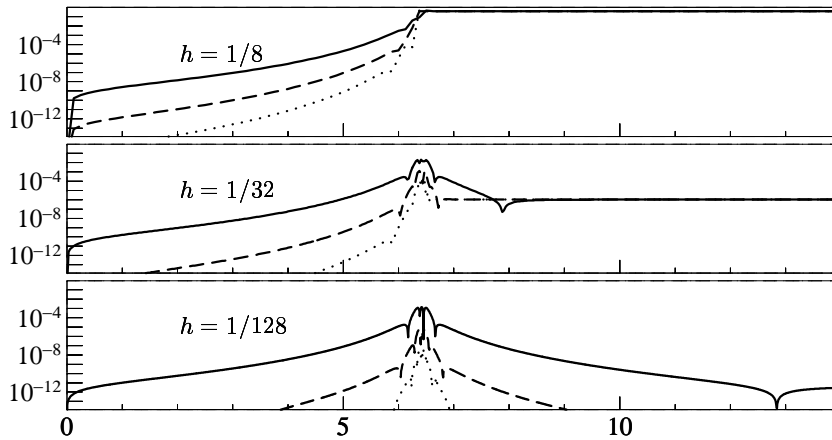
Fig. 1.4. Error in the truncated modified Hamiltonian for the Lennard–Jones potential and the Störmer–Verlet method.

The solid lines in Figure 1.4 show the error in the Hamiltonian $H(p,q)$ for the Störmer–Verlet method applied with 3 different step sizes. In the beginning this error is very small, then it increases and is maximal when the particle approaches the wall. At $t \approx 6.5$ the value of q is very small, so that the Lipschitz constant of the system (i.e., ω in (1.11)) is large. For relatively large step sizes h (upper pictures of Figure 1.4) when $\omega h \approx 1$, the exponential term in (1.11) becomes dominant, and energy conservation breaks down. In such situations, the value of the energy can change dramatically. We thus see that in spite of the use of a symplectic integrator, the energy drifts off the correct value if the step size is too large.

For this simple problem, we have computed the perturbations $H_3(y)$ and $H_5(y)$ in the modified Hamiltonian (the functions $H_{2k}(y)$ vanish identically, because the Störmer–Verlet method is symmetric). In Figure 1.4 we have included the functions $H(y_n) + h^2 H_3(y_n) - const$ (dashed) and $H(y_n) + h^2 H_3(y_n) + h^4 H_5(y_n) - const$ (dotted), where the constants are chosen so that the expressions vanish at the initial value. We see that $H(y_n) + h^2 H_3(y_n) + h^4 H_5(y_n) = const$ up to round-off on a large part of the interval considered. This nicely illustrates that the modified Hamiltonian is much better conserved than the energy $H(y)$.

1.3 Methods that nearly conserve quadratic first integrals

We next study the question whether a larger class of numerical integra-
tors can have the same good energy conservation as symplectic methods.
Let us begin with an instructive example.

1.3.1 Trapezoidal rule

Consider the trapezoidal rule

$$y_{n+1} = y_n + \frac{h}{2}\Big(f(y_n) + f(y_{n+1})\Big), \qquad (1.14)$$

and apply it to the Sun–Jupiter–Saturn system as in the previous exper-
iments. Figure 1.5 shows the error in the Hamiltonian (upper picture)
and in the angular momentum (lower picture), which is a quadratic first
integral of the system. We have used the same initial data and the same
integration interval as in Figure 1.3, and constant step size $h = 50$.

We first notice that the trapezoidal rule cannot be symplectic. Oth-
erwise, by Theorem 1.2.1, the angular momentum would be exactly
conserved along the numerical solution. Nevertheless, we observe an
excellent conservation of the total energy, very similar to that for the
symplectic Euler method of Figure 1.3. We shall give two explanations
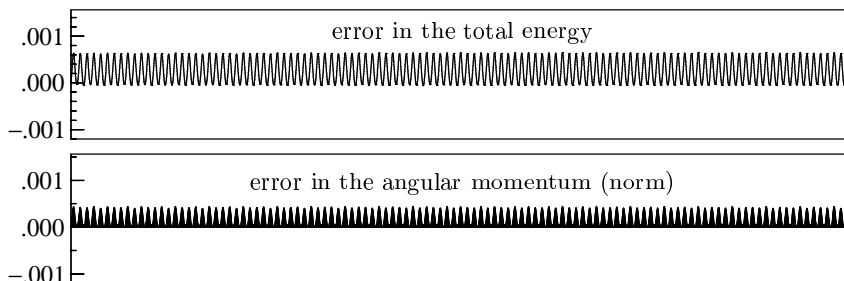of this good long-time behaviour.

Fig. 1.5. Error in the total energy and in the angular momentum for the
trapezoidal rule.

1st explanation: near-conservation of quadratic first integrals.
Let $u(t)$ be a solution of the modified differential equation in the sense
of backward error analysis, cf. (1.12). For the moment we only need that

$u(t)$ is smooth and $u(t_n) = y_n$. This function thus satisfies

$$u(t + h) = u(t) + \frac{h}{2}\Big(f\big(u(t + h)\big) + f\big(u(t)\big)\Big).$$

Writing the Taylor series expansion as $u(t + h) = \mathrm{e}^{hD}u(t)$, where D denotes differentiation with respect to time t, this relation becomes

$$\Big(\mathrm{e}^{hD} - 1\Big)u(t) = \frac{h}{2}\Big(\mathrm{e}^{hD} + 1\Big)f\big(u(t)\big) \tag{1.15}$$

or, equivalently,

$$\Big(1 - \frac{h^2}{12}D^2 + \frac{h^4}{120}D^4 + \dots\Big)\dot{u}(t) = f\big(u(t)\big). \tag{1.16}$$

Assume now that $Q(y) = y^T C y$ is a first integral of the differential equation (like the angular momentum in the Sun–Jupiter–Saturn system). This is equivalent to the condition $y^T C f(y) = 0$ for all y. Multiplying (1.16) from the left by $u(t)^T C$ gives a vanishing right-hand side and (omitting the obvious argument t)

$$u^T C\Big(\dot{u} - \frac{h^2}{12}\,u^{(3)} + \frac{h^4}{120}\,u^{(5)} + \dots\Big) = u^T C f(u) = 0. \tag{1.17}$$

Miraculously, this expression can be written as a total differential and, after multiplication by 2, becomes

$$\frac{d}{dt}\Big(u^T C u - \frac{h^2}{12}\big(2u^T C \ddot{u} - \dot{u}^T C \dot{u}\big) + \dots\Big) = 0. \tag{1.18}$$

This means that the function $u(t)$ and hence the numerical solution of the trapezoidal rule leaves the expression

$$\widetilde{Q}(y) = y^T C y - \frac{h^2}{12}\Big(2y^T C f'(y)f(y) - f(y)^T C f(y)\Big) + \dots \tag{1.19}$$

invariant. Consequently, the original first integral $Q(y) = y^T C y$ is nearly conserved with an $\mathcal{O}(h^2)$ error that does not grow with time. This completely explains the behaviour of the lower picture of Figure 1.5.

2nd explanation: conjugate symplecticity. Let Φ_h^{Eulex} and Φ_h^{Eulim} denote the numerical flow of the explicit and implicit Euler methods, respectively. Those of the trapezoidal rule (1.14) and of the midpoint rule (1.7) are then given by

$$\Phi_h^{\mathrm{trap}} = \Phi_{h/2}^{\mathrm{Eulim}} \circ \Phi_{h/2}^{\mathrm{Eulex}}, \qquad \Phi_h^{\mathrm{midp}} = \Phi_{h/2}^{\mathrm{Eulex}} \circ \Phi_{h/2}^{\mathrm{Eulim}}.$$

This implies that the trapezoidal rule and the implicit midpoint rule are connected by the conjugacy relation $\Phi^{\text{Eulex}}_{h/2} \circ \Phi^{\text{trap}}_h = \Phi^{\text{midp}}_h \circ \Phi^{\text{Eulex}}_{h/2}$. With $\chi_h := (\Phi^{\text{midp}}_h)^{-1/2} \circ \Phi^{\text{Eulex}}_{h/2}$, which is $\mathcal{O}(h^2)$ close to the identity,

$$\chi_h \circ \Phi^{\text{trap}}_h = \Phi^{\text{midp}}_h \circ \chi_h \quad \text{and} \quad \chi_h \circ (\Phi^{\text{trap}}_h)^n = (\Phi^{\text{midp}}_h)^n \circ \chi_h, \quad (1.20)$$

so that a numerical solution $\{y_n\}_{n\geq 0}$ of the trapezoidal rule is connected via $\chi_h(y_n) = z_n$ to the numerical solution $\{z_n\}_{n\geq 0}$ of the midpoint rule obtained with starting value $z_0 = \chi_h(y_0)$. This explains why the non-symplectic trapezoidal rule has the same good long-time behaviour as the symplectic midpoint rule (upper picture of Figure 1.5).

1.3.2 Symmetric linear multistep methods

Symmetric linear multistep methods form an important class of numerical integrators that have properties similar to those of the trapezoidal rule. However, one has to take care of the stability of parasitic solutions.

Multistep methods for first-order differential equations. Since the numerical solution of a multistep method

$$\alpha_k y_{n+k} + \ldots + \alpha_0 y_n = h\big(\beta_k f(y_{n+k}) + \ldots + \beta_0 f(y_n)\big) \qquad (1.21)$$

depends on k starting approximations $y_0, \ldots, y_{k-1}$, it is not at all obvious how symplecticity or the conservation of first integrals should be interpreted. The key idea is to consider the so-called *underlying one-step method* $\Phi_h(y)$, which is formally a series like (1.4), whose coefficients $a(\bullet)$, $a(\textit{\j})$, ... are determined by

$$\alpha_k \Phi^k_h(y) + \ldots + \alpha_1 \Phi_h(y) + \alpha_0 y = h\big(\beta_k f(\Phi^k_h(y)) + \ldots + \beta_0 f(y)\big).$$

This means that for starting approximations given by $y_j = \Phi^j_h(y_0)$ for $j = 0, \ldots, k-1$, the numerical solutions of the multistep method and of its underlying one-step method are identical. We say that the linear multistep method (1.21) is symplectic (conserves energy, conserves quadratic first integrals, ...), if its underlying one-step method is symplectic (conserves energy, conserves quadratic first integrals, ...).

It has been shown by Tang (1993) that linear multistep methods cannot be symplectic. However, they have an interesting property that will be explained next. If we let $u(t)$ be the solution of the modified differential equation of $\Phi_h(y)$, we have

$$\rho(\mathrm{e}^{hD})u(t) = h\sigma(\mathrm{e}^{hD})f\big(u(t)\big),$$

where $\rho(\zeta)$ and $\sigma(\zeta)$ are the generating polynomials of the coefficients α_j and β_j, respectively. This equation reduces to (1.15) for the trapezoidal rule. If the method is symmetric ($\alpha_{k-j} = -\alpha_j$ and $\beta_{k-j} = \beta_j$), the analysis of Section 1.3.1 extends straight-forwardly to the present situation, and shows that for problems having $Q(y) = y^T C y$ as first integral there exists $\widetilde{Q}(y)$ of the form (1.19) which is exactly conserved by the method (see Hairer & Lubich (2004)). Moreover, Chartier, Faou & Murua (2005) have shown that a method with this property is conjugate to a symplectic integrator.

Attention! In spite of these nice properties of symmetric linear multistep methods (1.21), they are not recommended for the long-time integration of Hamiltonian systems. The difficulty is that for nonlinear problems no results on stable propagation of the parasitic solution components are known, and numerical experiments reveal that they are unstable in most cases.

Multistep methods for second-order differential equations. An important class of Hamiltonian systems have $H(p, q) = \frac{1}{2}p^T M^{-1} p + U(q)$ with constant mass matrix M (for convenience we assume in the following that M is the identity). Such problems are equivalent to the second-order differential equation

$$\ddot{q} = -\nabla U(q), \qquad (1.22)$$

and it is natural to consider multistep methods adapted to this form:

$$\alpha_k q_{n+k} + \ldots + \alpha_0 q_n = -h^2\big(\beta_k \nabla U(q_{n+k}) + \ldots + \beta_0 \nabla U(q_n)\big). \quad (1.23)$$

Notice that the Störmer–Verlet method (1.10) is a special case of this formulation. The statements for methods (1.21) can all be extended to the situation of second-order differential equations (near conservation of quadratic first integrals, conjugate symplecticity of the underlying one-step method).

To also obtain bounds on the parasitic solution components for arbitrary starting approximations, we extend the idea of backward error analysis (Hairer 1999). We write the numerical solution as

$$q_n = v(nh) + \sum \zeta_j^n w_j(nh) \qquad (1.24)$$

where the ζ_j's stand for zeros (different from 1) of the characteristic polynomial $\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j$ and products thereof. Inserting (1.24) into the linear multistep formula (1.23), expanding into a Taylor series,

and comparing the expressions multiplying ζ_j^n and powers of h, we get the modified equations – a second-order differential equation for $v(t)$, first-order differential equations for $w_j(t)$ if ζ_j is a simple zero of $\rho(\zeta)$, and algebraic relations, if ζ_j is a product of zeros of $\rho(\zeta)$.

If we are interested in energy conservation we have to complement (1.23) with an approximation of the derivative, which in general is given by a formula of the form

$$\dot{q}_n = \frac{1}{h} \sum_{j=-\ell}^{\ell} \delta_j q_{n+j}.$$

Exploiting the Hamiltonian structure in the modified differential equations, Hairer & Lubich (2004) prove the following result.

Theorem 1.3.1 *Consider the Hamiltonian system (1.22) with analytic potential function $U(q)$, and assume that the linear multistep method (1.23) has order r and is*

- *symmetric, i.e., $\alpha_{k-j} = \alpha_j$ and $\beta_{k-j} = \beta_j$;*
- *without weak instability, i.e., $\rho(\zeta) = (\zeta - 1)^2 \widehat{\rho}(\zeta)$ and the zeros of $\widehat{\rho}(\zeta)$ lie on the unit circle, are simple, and different from 1.*

If the starting approximations $q_0, \ldots, q_{k-1}$ are $\mathcal{O}(h^{r+1})$ close to the exact solution, and the numerical solution stays in a compact set, then we have on intervals of length $T = \mathcal{O}(h^{-r-2})$

- $\|w_j(t)\| \leq Ch^{r+1}$ *with C independent of t;*
- $\{q_n, \dot{q}_n\}$ *nearly conserves the total energy (without drift);*
- $\{q_n, \dot{q}_n\}$ *nearly conserves quadratic first integrals of the form $q^T E \dot{q}$ (without drift).*

We do not have energy conservation on exponentially long time intervals (as for symplectic integrators), but the intervals are sufficiently long for practical computations. This result justifies the use of high-order symmetric linear multistep methods (1.23) for long-time integrations in celestial mechanics.

1.4 Energy conservation with symmetric methods

There is still another class of numerical integrators – symmetric methods – which, for special kinds of Hamiltonian systems, give good energy conservation. Since in certain situations (such as variable step size integration, multiple time stepping, reversible averaging) it is much easier
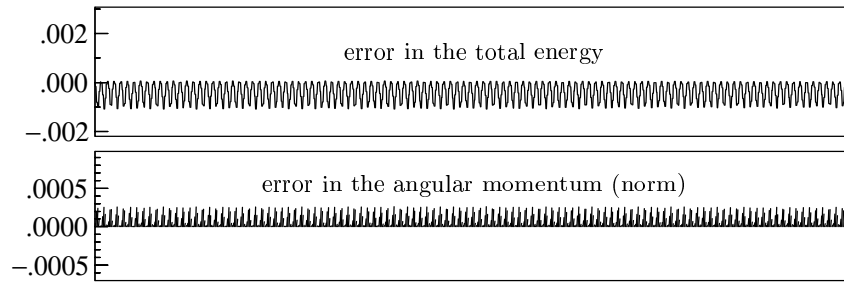
Fig. 1.6. Error in the total energy and in the angular momentum for the 3-stage Lobatto IIIB method.

to design symmetric discretisations than symplectic ones, it is of interest to characterise the problems for which symmetric methods have a good long-time behaviour.

1.4.1 Symmetric non-symplectic methods

Let us start with a numerical experiment. We consider the 3-stage Lobatto IIIB method which is an implicit Runge–Kutta method (its coefficients can be found in Section II.1.4 of HLW02). It is neither symplectic nor conjugate to a symplectic method (see Section VI.7.4 of HLW02), but it is a symmetric integrator. This means that its numerical flow satisfies $\Phi_{-h}^{-1}(y) = \Phi_h(y)$. We apply this integrator with step size $h = 400$ in the usual way to the three-body Sun–Jupiter–Saturn system. The result can be seen in Figure 1.6. There is apparently no difference compared with the results obtained by the trapezoidal rule. What is the reason?

1.4.2 Integrable reversible systems

Unfortunately, very little is known about the energy conservation of symmetric B-series methods. The only exceptions are integrable reversible systems. In this survey article we present some results without giving all the technical assumptions, and we refer the interested reader to Chapter XI of HLW02.

We assume that the differential equation (not necessarily Hamiltonian) can be written in the form

$$\dot{u} = f(u, v), \qquad \dot{v} = g(u, v), \tag{1.25}$$

and that it is *reversible* with respect to the involution $(u, v) \mapsto (u, -v)$. This means that

$$f(u, -v) = -f(u, v), \qquad g(u, -v) = g(u, v). \qquad (1.26)$$

Hamiltonian systems, for which the Hamiltonian is quadratic in p, satisfy these relations with q in the role of u, and p in the role of v.

Such a system is called an *integrable reversible system* if there exists a reversibility-preserving change of coordinates $(a, \theta) \mapsto (u, v)$ such that in the new coordinates the system is of the form

$$\dot{a} = 0, \qquad \dot{\theta} = \omega(a). \qquad (1.27)$$

This system can be solved exactly. The *action* variables a are constant (i.e., first integrals), and the *angle* variables θ grow linearly with time. The Kepler problem with $H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - (q_1^2 + q_2^2)^{-1/2}$ satisfies all these conditions if we put $u = (q_1, p_2)$ and $v = (-p_1, q_2)$. The Sun–Jupiter–Saturn system is a small perturbation of an integrable reversible system.

Under certain technical assumptions (analyticity of the vector field, strong non-resonance condition, etc.) it is proved in HLW02 that all action variables are nearly conserved over long times for symmetric B-series methods. Moreover, the global error grows at most linearly with time. Since these results hold also for small reversible perturbations of integrable reversible systems, the behaviour shown in Figure 1.6 is explained.

1.4.3 An example: the perturbed pendulum

Let us illustrate with a simple example the difficulties that can be encountered by a symmetric method. Consider the one-degree-of-freedom Hamiltonian system with (see Figure 1.7)

$$H(p, q) = \frac{1}{2}\, p^2 - \cos q + 0.2 \sin(2q). \qquad (1.28)$$

With $u = q$ and $v = p$ it is of the form (1.25) and satisfies the condition (1.26). Considered as a Hamiltonian system, it is also integrable.

We consider two different initial values (thick points in Figure 1.7). The values $q_0 = 0$ and $p_0 = 1.8$ produce a periodic solution whose orbit is invariant with respect to the reflection $p \mapsto -p$. For $q_0 = 0$ and $p_0 = 2.2$ the solution is still periodic (on the cylinder), but it does not contain any symmetry.
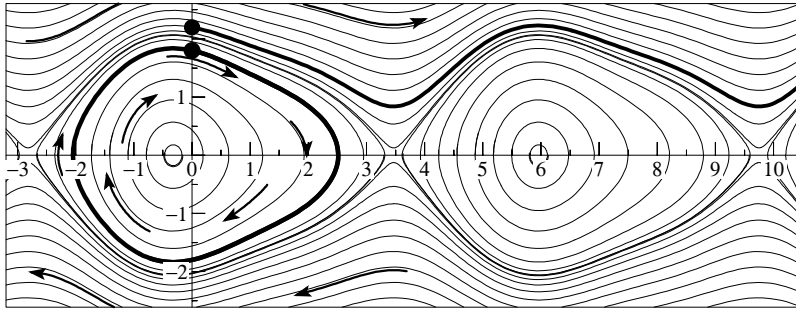
Fig. 1.7. Phase portrait of the perturbed pendulum problem.

As in the previous experiment, we apply the 3-stage Lobatto IIIB method. We use the step size $h = 0.2$ and consider an interval of length 200. For the initial values with symmetric solution (Figure 1.8) the energy is well conserved without any drift. For the second set of initial values, however, there is a clear drift in the energy along the numerical solution (Figure 1.9).

Symplectic methods and methods that are conjugate to a symplectic method will have bounded energy error for this problem. We have
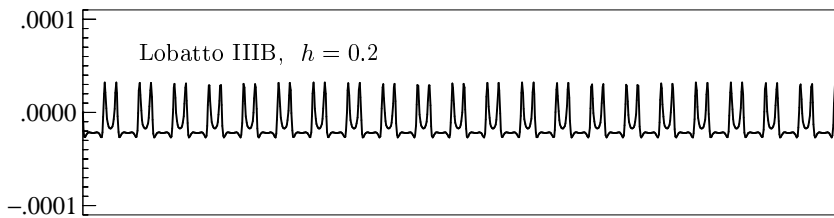

Fig. 1.8. Energy conservation of the Lobatto IIIB method for the perturbed pendulum with initial values corresponding to a symmetric solution.
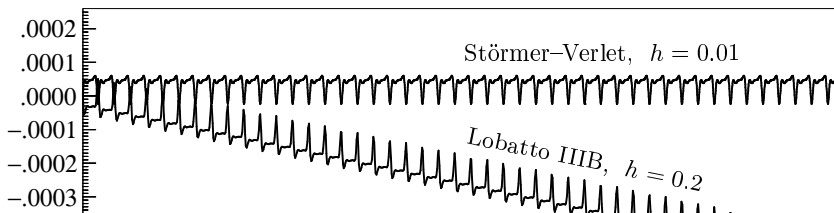

Fig. 1.9. Energy conservation of the Lobatto IIIB method for the perturbed pendulum with initial values corresponding to a solution without symmetry. The result of the symplectic Störmer–Verlet scheme is included.

included in Figure 1.9 the numerical result obtained with the symplectic Störmer–Verlet method (with smaller step size, because it is only of order 2, compared to order 4 of the Lobatto IIIB method).

1.5 Concluding remarks

In many applications, and in particular in long-time integrations of mechanical systems, it is important that the energy along the numerical solution does not drift from the correct value. Within the class of B-series methods we have studied the following properties:

- *symplecticity (Section 1.2):* the energy is nearly conserved for all Hamiltonian systems (integrable or chaotic) provided the step size is sufficiently small;
- *conjugate symplecticity (Section 1.3):* methods with this property have the same long-time behaviour as symplectic methods and are well suited for the integration of Hamiltonian systems;
- *symmetry (Section 1.4):* for reversible Hamiltonian systems and a solution with a certain symmetry, symmetric methods usually give excellent results; a complete explanation is missing in many situations.

Figure 1.10 shows the connections between these properties. Symplecticity and exact energy conservation are not compatible. However, it is possible to have symmetric methods that exactly conserve energy. Examples are energy-momentum methods (see Section V.5 of HLW02) which, however, do not fall into the class of B-series methods.
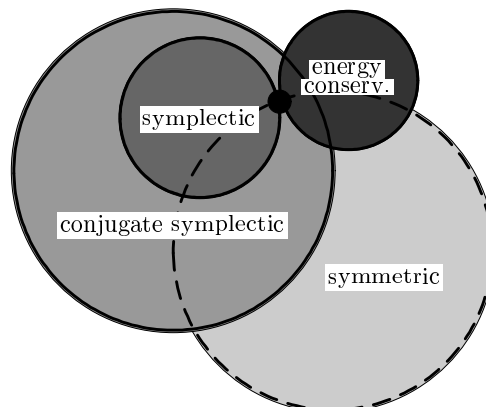

Fig. 1.10. Survey of geometric integrators for Hamiltonian systems.

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